

Dynamic Correlators of FPU Chains and Nonlinear Fluctuating Hydrodynamics

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We study the equilibrium time correlations for the conserved fields of classical anharmonic chains and argue that their dynamic correlator can be predicted on the basis of nonlinear fluctuating hydrodynamics. In fact our scheme is more general and would cover also other one-dimensional hamiltonian systems, for example classical and quantum fluids. The only input parameters required are the average equilibrium currents and the static susceptibilities of the conserved fields. In our context fluctuating hydrodynamics is a nonlinear system of conservation laws with noise. For a single mode it is equivalent to the noisy Burgers equation, for which explicit solutions are available. Our focus is the case of several modes. No exact solutions have been found so far and we rely on a one-loop approximation. The resulting mode-coupling equation has a quadratic memory kernel and describes the time evolving correlator matrix of all locally conserved fields. Long time asymptotics is computed analytically and finite time properties are obtained through a numerical simulation of the mode-coupling equations, which provide predictions still to be compared with data from molecular dynamics.

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To predict the dynamic correlator of anharmonic chains is still a theoretical challenge. In higher dimensions fluctuating hydrodynamics serves as a convenient starting point [1–3]. But, as recognized already in the 1970ies [4, 5], in one dimension, while the static correlations are of short range, the dynamic current-current correlations generically have an anomalously slow decay. In particular the transport coefficients, required as an input for fluctuating hydrodynamics, are no longer properly defined. There have been huge efforts, both through theoretical investigations and numerical simulations, to more precisely characterize this “anomalous” behavior (for a partial list on FPU chains only, see [6–11]). Here we argue that, in one dimension, linear fluctuating hydrodynamics has to be extended to a *nonlinear* version, which will be outlined below. There have been related attempts before [12, 13]. Our main advance is to treat the full system of coupled conserved modes and to run time-dependent numerical simulations of the respective mode-coupling equations. In the simulation we use the exact, microscopically computed parameters for the particular anharmonic chain under consideration and thereby provide time-resolved predictions which can be compared directly with the corresponding molecular dynamics.

As a start-up, let us recall the case of a single conserved field, say $\tilde{u}(x, t)$, space $x \in \mathbb{R}$, time t , which satisfies the conservation law

$$\partial_t \tilde{u}(x, t) + \partial_x j(\tilde{u}(x, t)) = 0 \quad (1)$$

with given current function $j(\tilde{u})$. We want to study the fluctuations relative to a uniform background \mathbf{u} , i.e. $\tilde{u}(x, t) = \mathbf{u} + u(x, t)$, hence expand (1) to *second* order and add dissipation and noise,

$$\partial_t u + \partial_x (j'(\mathbf{u})u + \tfrac{1}{2}j''(\mathbf{u})u^2 - D\partial_x u + \sqrt{\sigma}\xi) = 0, \quad (2)$$

where $\xi(x, t)$ is normalized space-time white noise. We consider the mean zero, space-time stationary process $u(x, t)$ governed by (2). Then the spatial statistics at fixed time t is white noise, $\langle u(x, t)u(x', t) \rangle = \chi\delta(x - x')$, $\chi = \sigma/2D$, which reflects that the static correlations of an underlying microscopic model decay exponentially fast. Of particular interest is the correlator $S(x, t) = \langle u(x, t)u(0, 0) \rangle$, $S(x, 0) = \chi\delta(x)$. Its large scale behavior will be dominated by the nonlinearity, but dissipation and noise is required to maintain the proper steady state. (2) is the noisy Burgers equation, equivalently the spatial derivative of the one-dimensional KPZ equation [14]. There is an exact computation of $S(x, t)$ using

replica [15]. In particular one knows the universal long time limit,

$$S(x, t) = \chi(\lambda_B |t|)^{-2/3} f_{\text{KPZ}}((\lambda_B |t|)^{-2/3}(x - j'(\mathbf{u})t)), \quad (3)$$

valid for large x, t , with $\lambda_B^2 = 2\chi j''(\mathbf{u})^2$. Identical scaling properties have been derived also for stochastic lattice gases [16, 17]. The universal scaling function f_{KPZ} can be written in terms of a Fredholm determinant and has been computed with great precision [18]. Because of the nonlinearity the spreading is faster than diffusive. On the other hand D, σ appear in (3) only through the static covariance χ . This quantity will have to come from the microscopic model, while dissipation and noise by themselves are phenomenological, not directly identifiable with microscopic properties. (3) and similar type of predictions based on (2) have been confirmed experimentally using a thin film of turbulent liquid crystal [19] and in Monte Carlo simulations of Eden cluster growth [20]. These results provide an indirect confirmation that higher order nonlinearities, like u^3 , will not change the scaling asymptotics.

Anharmonic chains have three conservation laws, compression (or elongation), momentum, and energy. Thus we have to extend the previous considerations to several modes (or components). We use α as mode index. Then (1) generalizes to

$$\partial_t \tilde{u}_\alpha + \partial_x j_\alpha(\vec{u}) = 0, \quad \alpha = 1, \dots, n, \quad (4)$$

$\vec{u} = (u_1, \dots, u_n)$. Expanding as $\tilde{u}_\alpha = \mathbf{u}_\alpha + u_\alpha$, the coefficients of the linearized equation are

$$A_{\alpha\beta}(\vec{u}) = \partial_{u_\beta} j_\alpha(\vec{u}) \quad (5)$$

and coefficients of the quadratic part are given by the Hessians

$$H_{\beta\gamma}^\alpha(\vec{u}) = \partial_{u_\beta} \partial_{u_\gamma} j_\alpha(\vec{u}). \quad (6)$$

Since the background \vec{u} is fixed, it will be suppressed in our notation. The equal time equilibrium correlations decay rapidly. Hence $u_\alpha(x, t)$ at fixed t is modeled as white noise with covariance $\langle u_\alpha(x, t) u_\beta(x', t) \rangle = C_{\alpha\beta} \delta(x - x')$. $C_{\alpha\beta} = C_{\beta\alpha}$ and $C > 0$ as a matrix. As only microscopic input, nonlinear hydrodynamics requires the currents j_α , more precisely A, H^α , and the static correlator C . As can be verified directly, for anharmonic chains it holds

$$AC = CA^\dagger \quad (7)$$

with ‘t’ denoting transpose. Hence A has a system of right and left eigenvectors, $A\psi_\alpha = c_\alpha\psi_\alpha$, $A^t\tilde{\psi}_\alpha = c_\alpha\tilde{\psi}_\alpha$, and it is convenient to switch to normal modes. We form the matrices $R = (\langle\tilde{\psi}_\alpha|)_{\{\alpha=1,\dots,n\}}$, $R^{-1} = (|\psi_\alpha\rangle)_{\{\alpha=1,\dots,n\}}$. Up to a global sign the eigenvectors are unique when normalized such that $RR^{-1} = 1$, $RCR^t = 1$. Then $RAR^{-1} = \text{diag}(c_1, \dots, c_n)$ and the normal modes, ϕ_α , are defined through $\vec{\phi} = A\vec{u}$. While not strictly necessary, the linear transformation to normal modes is of advantage, since normal modes have a definite propagation velocity and turn out to be essentially uncorrelated.

We now expand (4) to second order in \vec{u} , transform to normal modes, and add dissipation and noise with the result

$$\partial_t\phi_\alpha + \partial_x(c_\alpha\phi_\alpha + \sum_{\beta,\gamma=1}^n G_{\beta\gamma}^\alpha\phi_\beta\phi_\gamma - \partial_x(D\phi)_\alpha + \xi_\alpha) = 0, \quad (8)$$

where $G_{\beta\gamma}^\alpha = \frac{1}{2} \sum_{\alpha'} R_{\alpha\alpha'} \langle\psi_\beta|H^{\alpha'}\psi_\gamma\rangle$. The diffusion matrix D is positive definite. $\xi_\alpha(x, t)$ is space-time white noise with strength

$$\langle\xi_\alpha(x, t)\xi_\beta(x', t')\rangle = 2D_{\alpha\beta}\delta(x - x')\delta(t - t'). \quad (9)$$

As before, we consider the mean zero, stationary process $\vec{\phi}(x, t)$ governed by (8). In the linear case, $G = 0$, $\vec{\phi}(x, t)$ is a Gaussian process, which for fixed t has white noise statistics with independent components of unit strength as required by $RCR^t = 1$. It can be checked that, for a suitable spatial discretization of (8), this measure remains invariant under the full nonlinear evolution, provided the couplings $G_{\beta\gamma}^\alpha$ are symmetric in all indices [21]. In general, we assume that the steady state of (8) has short range correlations.

On the basis of (8) one would like to compute the dynamic correlator

$$S_{\alpha\beta}(x, t) = \langle\phi_\alpha(x, t)\phi_\beta(0, 0)\rangle, \quad (10)$$

which would serve then as an approximation to the true dynamic correlator of the microscopic model. Because of the nonlinearity, this is a difficult program and we rely here on a mode-coupling equation resulting from the one-loop expansion of (8). The precise details of the computation can be found elsewhere [21]. In essence, one writes down the evolution equation for $S_{\alpha\beta}(x, t)$, once iterated in time, which yields a time integral over the Gaussian propagator and an expectation of the form $\langle\phi(s)\phi(s)\phi(0)\phi(0)\rangle$ for the intermediate time s , $0 \leq s \leq t$. The Gaussian propagator is replaced by the full propagator and the 4-point

correlation is replaced by its Gaussian pairings, where the equal time pairing vanishes because of the conservation law and the remaining two pairings yield the same contribution. The result is a cubic memory equation. Anticipating already the application to anharmonic chains with integer particle index, numerically we use a unit spatial grid. Adopting the standard conventions for discrete Fourier transforms, in Fourier space the mode-coupling equation reads

$$\begin{aligned} \partial_t \hat{S}_{\alpha\beta}(k, t) = & -i c_\alpha \sin(2\pi k) \hat{S}_{\alpha\beta}(k, t) \\ & - 2(1 - \cos(2\pi k)) \sum_{\alpha'=1}^n \left(-D_{\alpha\alpha'} \hat{S}_{\alpha'\beta}(k, t) + \int_0^t ds \hat{M}_{\alpha\alpha'}(k, s) \hat{S}_{\alpha'\beta}(k, t-s) \right), \end{aligned} \quad (11)$$

$k \in [-\frac{1}{2}, \frac{1}{2}]$, with the quadratic memory kernel

$$\hat{M}_{\alpha\alpha'}(k, t) = 2 \sum_{\beta, \beta', \gamma, \gamma'=1}^n G_{\beta\gamma}^\alpha G_{\beta'\gamma'}^{\alpha'} \int_{-1/2}^{1/2} dq \hat{S}_{\beta\beta'}(k-q, t) \hat{S}_{\gamma\gamma'}(q, t), \quad (12)$$

which has to be solved with the initial condition

$$\hat{S}_{\alpha\beta}(k, 0) = \delta_{\alpha\beta}. \quad (13)$$

(11) is a lowest order approximation. However, for $n = 1$, first written down in [22], the exact solution (2) can be compared with the numerical solution of (11), (12). In Fig. 1 we display a time sequence for a single mode, $n = 1$, with $G_{11}^1 = \frac{1}{2}$. For $t \gtrsim 32$ the scaled solution remains stationary. We compare with the universal KPZ scaling function, thereby reproducing Fig. 3 of [23]. The asymptotic scaling function differs from f_{KPZ} by a few percent only. We expect that such a precision extends to several modes.

Numerically one observes that, while off-diagonal elements of $S_{\alpha\beta}$ develop immediately, they decay fairly rapidly. Thus we may invoke the diagonal approximation, $S_{\alpha\beta}(x, t) \simeq \delta_{\alpha\beta} f_\alpha(x, t)$ in position space, and the memory kernel becomes

$$M_{\alpha\alpha}(x, t) = 2 \sum_{\beta, \gamma=1}^n (G_{\beta\gamma}^\alpha)^2 f_\beta(x, t) f_\gamma(x, t). \quad (14)$$

Let us assume that all velocities $\{c_\alpha\}$ are distinct. Then, ignoring nonlinearities, the mode f_α is sharply peaked at $c_\alpha t$ and the modes separate from each other linearly in t . Hence the product $f_\beta f_\gamma$ decays rapidly, unless $\beta = \gamma$, and the off-diagonal terms in the sum (14) can be discarded. In general, two distinct scenarios may occur. (i) $G_{\alpha\alpha}^\alpha \neq 0$. Then $G_{\alpha\alpha}^\alpha f_\alpha f_\alpha$

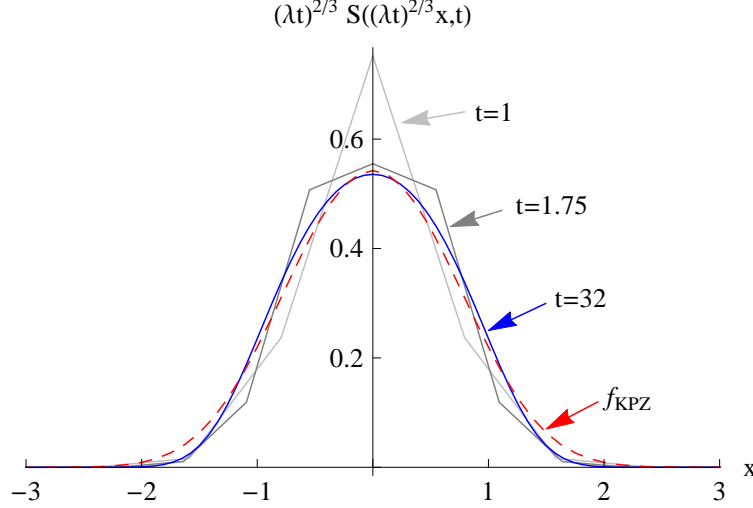


FIG. 1. (Color online) Time sequence of the numerical mode-coupling solution, $n = 1$, $G_{11}^1 = \frac{1}{2}$, rescaled by $(\sqrt{2}t)^{2/3}$. The curves are piecewise-linear due to the underlying spatial lattice. The exact KPZ scaling function is shown in dashed red.

travels with the same velocity as f_α and dominates the interaction with the other modes. The dynamics of the mode f_α reduces to the case $n = 1$ with scaling (2) and shift $c_\alpha t$. This is the KPZ dominated behavior. (ii) $G_{\alpha\alpha}^\alpha = 0$. The leading term vanishes and long time behavior is dominated by $G_{\beta\beta}^\alpha \neq 0$. If also $G_{\beta\beta}^\beta \neq 0$, then the coupling of mode α to the pair of modes β results in a scaling function $\hat{f}_\alpha(k, t) = \exp[-|k|^{5/3}|\lambda_h t|]$ with computable coefficient λ_h , see [21].

There are more cases to be considered, but equipped with this nonlinear extension of fluctuating hydrodynamics it is more interesting to understand how one obtains a prediction for the structure factor of anharmonic chains. We first have to figure out the conserved fields and their macroscopic Euler equations. The chain consists of N particles, position q_j , momentum p_j , $j = 1, \dots, N$, unit mass, and is governed by the hamiltonian

$$H = \sum_{j=1}^N \left(\frac{1}{2} p_j^2 + V(q_{j+1} - q_j) \right), \quad (15)$$

where periodic boundary conditions, $q_{N+1} = q_1 + L$, are imposed. A prototypical potential is the FPU choice $V(y) = \frac{1}{2}y^2 + \frac{1}{3}ay^3 + \frac{1}{4}y^4$. The locally conserved microscopic fields are compression $r_j = q_{j+1} - q_j$, momentum p_j , and energy $e_j = \frac{1}{2}p_j^2 + V(r_j)$. In a microcanonical simulation one fixes the length (compression) per particle, ℓ , as $L = N\ell$, the momentum per particle, u , as $\sum_{j=1}^N p_j = Nu$, and the energy per particle, ϵ , as $H = N\epsilon$. Computationally,

it is convenient to switch to the grand canonical pressure ensemble. Then ℓ is paired with the pressure p and the internal energy \mathfrak{e} with the inverse temperature β . In the grand canonical ensemble, $\{r_j, p_j\}$ become independent random variables. The distribution of p_j is a Maxwellian shifted by \mathbf{u} , and the distribution of r_j is given by $Z^{-1} \exp[-\beta(V(y) + py)] = \langle \cdot \rangle_{p,\beta}$ with partition function $Z = \int dy \exp[-\beta(V(y) + py)]$. Clearly the pressure is just the average force acting on a specified particle. The microcanonical and grand canonical parameters are related through

$$\ell = \langle y \rangle_{p,\beta}, \quad \mathfrak{e} = \frac{1}{2\beta} + \langle V(y) \rangle_{p,\beta}. \quad (16)$$

The hydrodynamic currents are

$$j_\ell = -\mathbf{u}, \quad j_u = p(\ell, \mathfrak{e} - \tfrac{1}{2}\mathbf{u}^2), \quad j_\mathfrak{e} = \mathbf{u}p(\ell, \mathfrak{e} - \tfrac{1}{2}\mathbf{u}^2), \quad (17)$$

which inserted in (4) result in the Euler hydrodynamics of the anharmonic chain. Note that variable x corresponds to the continuum approximation of the particle index.

Without loss of generality we expand at $\mathbf{u} = 0$. All coupling coefficients appearing in (12) can be computed in terms of at most third order cumulants involving $y, V(y)$. These integrals and the somewhat unwieldy substitutions are easily performed using Mathematica. There are three modes: the heat mode, $\alpha = 0$, with velocity $c_0 = 0$ and two sound modes, $\alpha = \pm 1$, with velocity $c_\sigma = \sigma c$, $\sigma = \pm 1$, where c is the sound speed,

$$c^2 = -\partial_\ell p + p \partial_\mathfrak{e} p. \quad (18)$$

Since momentum is conserved, $H_{\alpha\beta}^\ell = 0$. Most importantly $G_{00}^0 = 0$, always. Hence the heat mode is predicted to have non-KPZ scaling. A particular and much studied case is an even potential, $V(y) = V(-y)$, at $p = 0$. Then many cumulants vanish. In fact the only non-zero coefficients are $G_{0\pm}^\pm$ and G_{++}^0, G_{--}^0 . On this basis one expects the sound modes to be diffusive and the feed-back on the heat mode to lead to the scaling function $\hat{f}_0(k, t) = \exp[-|k|^{3/2} \lambda_h |t|]$.

To go beyond the large t asymptotics we turn to the simulation of the mode-coupling equations, which is based on the Fourier space representation (11), in such a way that the values of the memory kernel $\hat{M}_{\alpha\alpha'}(k, s)$ for $s < t$ can be stored and re-used. The time and momentum variables are discretized by a uniform grid. The parameters of the chain are picked somewhat arbitrarily but related to the parameters used in molecular dynamics

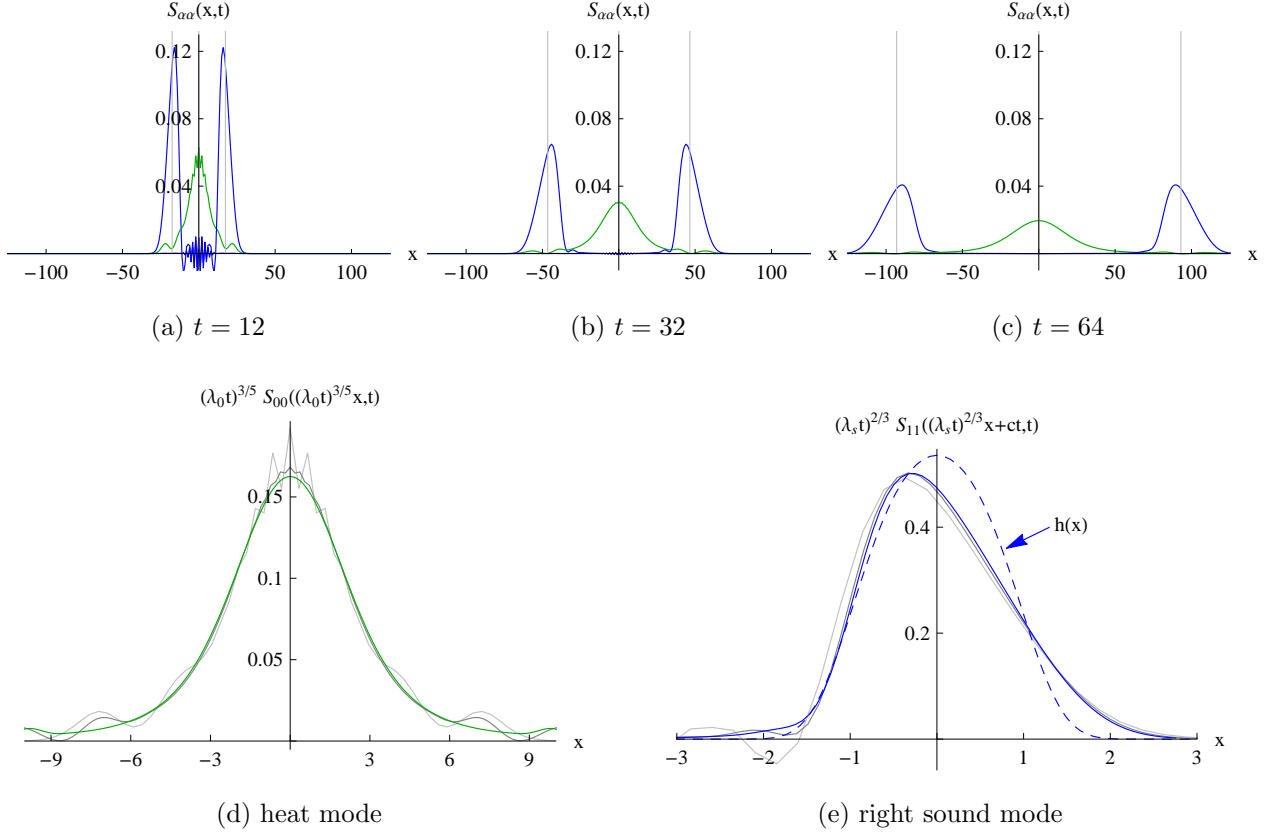


FIG. 2. (Color online) Time sequence of normal mode correlations for the FPU chain with $\mathbf{a} = 2$, $p = 1$, $\beta = 0$, and $\mathbf{u} = 0$ (a), (b), (c). Magnification of the central heat mode peak (d) and the right sound mode peak (e) in suitably rescaled coordinates.

[9, 10]. We stress that simulations can be performed for any choice of the potential and thermodynamic parameters at minimal numerical efforts. Fig. 2 is obtained for the FPU potential with $\mathbf{a} = 2$ and $\mathbf{u} = 0$, $p = 1$, $\beta = 2$, resulting in $c = 1.455$. $V(y) + py$ has a single critical point at $y = -1.755$. The grey vertical lines at $\pm ct$ indicate the predicted position of the sound mode peaks. In the time sequence we display the superimposed normal mode correlations (area 1 under each curve). More details are provided in the blow-up. For the heat mode one observes oscillations which move away from the center and eventually die out. The tail of the heat mode is cut off at the location of the sound mode, but in-between the two sound mode peaks the theoretically predicted curve is approached. At the longest available time the sound modes are still asymmetric and have not yet reached their asymptotic shape.

Based on these and further simulations of the mode-coupling equations for anharmonic chains, the following qualitative picture for the motion of the peaks in index number space

seems to emerge. The sound modes “rapidly” decay to a shape function which is centered at σct and varies on the scale $t^{2/3}$. The shape function itself is still slowly varying. The coupling $G_{\sigma\sigma}^0$ determines the scaling of the heat mode. Since only the integral over the square of the shape function is involved, the heat mode rapidly achieves its asymptotic form in the range $\{|x| \leq ct\}$ and with a still slowly varying non-universal constant. The slow motion of the sound modes is governed by G_{00}^σ and $G_{-\sigma-\sigma}^\sigma$. Assuming already the overall scaling picture, the size of these corrections is estimated to be of the order $t^{-1/15}$, resp. $t^{-1/9}$, relative to the leading term which indicates that f_{KPZ} is approached rather slowly. Of course, only a guideline can be presented. For the precise dynamics all couplings have to be used.

Conclusions. We developed a nonlinear extension of fluctuating hydrodynamics applicable to one-dimensional systems, in principle including classical fluids, quantum fluids [24–26], and quantum spin chains. Already at the level of the one-loop approximation it is crucial to maintain the couplings between all conserved modes. Numerical solutions of the mode-coupling equations provide a realistic picture of the correlation dynamics. On the limited time scale available, the numerical solutions are in agreement with the analytical computations. But the theory still has to pass the key test, namely a quantitative comparison with molecular dynamics. In this test one has to keep in mind that nonlinear fluctuating hydrodynamics is itself an approximation at best valid only for long times and wavelengths. In addition mode-coupling is an approximation to nonlinear fluctuating hydrodynamics, albeit likely to be fairly accurate, as demonstrated in Fig. 1

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